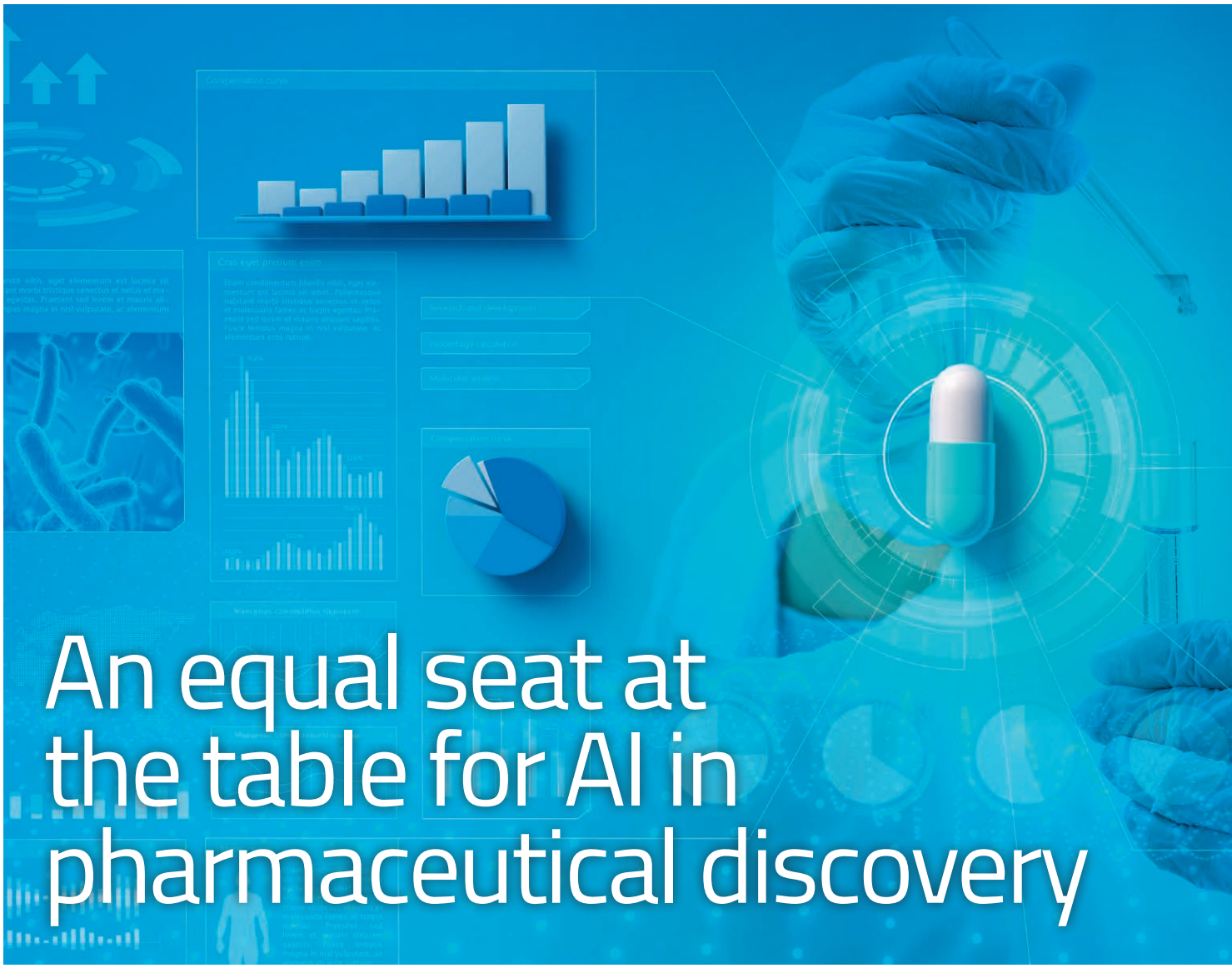

An equal seat at the table for AI in pharmaceutical discovery

This article explores the current state of artificial intelligence (AI) in drug discovery and development, discussing the obstacles holding back wider adoption. Dr Mark Eller, Senior Vice President of Research and Development at Aria Pharmaceuticals, makes the case that to succeed, AI must be integrated as a partner alongside core pharmaceutical R&D disciplines.

AS A FORMER R&D lead, my perspective was not unlike many. After being so immersed in the process of discovering and developing new drugs using traditional methods and practices, it was difficult for me to wrap my mind around a reality where AI could replace all the hard work and research of humans to produce the same product, much less produce it significantly faster.

Afterall, my background is in drug discovery and development; an industry driven by rigorous science where shortcuts are not an option. I helped lead R&D programmes that introduced new and lifesaving treatments to millions of patients and the traditional process was working.

Today, that has significantly changed and now I see tremendous value in engaging technology – more specifically, AI – as a valuable R&D partner. Our access to powerful computational tools and machine learning has the potential to revolutionise the industry, promising to help scientists find new breakthroughs faster and with more certainty of success. Discussions about technology and AI related to accelerating drug discovery have been significant in the past several years. The barriers and relevant solutions to digital transformation are plentiful, ranging from the availability of data to the very algorithms that drive the technology. While these are all important, the key word here is 'partner'

and a successful partnership requires active integration of technology into the process.

The use of technology and AI is currently unsystematic. Pilot programmes, bolt-on software approaches and outsourcing of drug discovery tasks to software-led companies are a norm in today's industry. The point is that much of the industry has dabbled in the use of advanced computational technology to support drug discovery, but very few have truly integrated its capabilities and elevated technology as a core discipline of research and discovery. So, what is holding us back?

The first major obstacle is education. Technology and AI have been developed and used for years in all industries. Today, our access to computational power has dramatically evolved and it has done so quickly. However, this swift evolution has led to insufficient education that is required to get the scientific community on board.

We must first understand that technology and AI were never meant to replace the scientists and medical experts working on new drugs. They are a toolset that can support scientific work and vice versa. Once again, it is a partnership. However, if technologists do not understand the role of biologists and vice versa, it creates a major disconnect. We must therefore find ways to better educate each side. Rather than hyping the technology, we can reframe the conversation to revolve around pragmatic education. »

"We must first understand that technology and AI were never meant to replace the scientists and medical experts working on new drugs"

EXPERT VIEW

Cathie Miller, PhD
Senior Director of Product Marketing, Personalized Medicine, BioIVT

BIOIVT
ELEVATING SCIENCE

For further information, visit:
www.bioivt.com

Supporting artificial intelligence and machine learning with biomedical data

The use of machine learning (ML) in drug discovery requires ample amounts of biomedical data. A defined cohort with verified and characterised data, along with integrated Hematoxylin and Eosin (H&E) images and associated data, supports artificial intelligence (AI) applications within target discovery/drug development workflows and digital pathology programmes.

For over 30 years, BioIVT has used rigorous QA standards to prospectively collect biospecimens for our ASTERAND® Human Tissue Repository, processing over one million specimens with high-quality, thoroughly characterised and validated data, including full-slide histological Aperio images. That data is now available for integration into ML workflows, supporting the discovery of patterns and relationships relevant to both disease etiology and pathology.

Our biospecimens are collected with comprehensive clinical data from each donor site. We follow a strict and standardised electronic record review process, where each individual tissue block is reviewed by independent, board-certified clinical pathologists to ensure correspondence with clinical information. Pathological data is classified using ICD codes as appropriate for anatomic site, morphology and behaviour, with World Health Organization (WHO) oncology classifications for tumour indications. When possible, we include outcome data, which is useful for target discovery and development-related ML.

Equally important is to have compliance with national, regional and local regulatory and ethical standards along with donor consent for use in a broad range of commercial products and services. At BioIVT, all human tissue samples are collected under IRB-approved protocols and are de-identified prior to banking and distribution, compliant with the US Health Insurance Portability and Accountability Act (HIPAA), the UK Human Tissue Authority (HTA) and accredited by the College of American Pathologists (CAP).

Regardless of the use, BioIVT's specimen database supports a diverse range of AI/ML applications.

"Improved education should prevent the hype and change the narrative over time"

Dr Mark Eller

Mark is Senior Vice President of Research and Development at Aria Pharmaceuticals. He has led teams from discovery through approval at several companies including Jazz Pharmaceuticals, Quintiles (now IQVIA) and HMR (now Sanofi). Mark is co-inventor on 30 patents and has led health authority presentations and negotiations, including six FDA advisory committee meetings. He has co-authored numerous scientific publications and served as an Adjunct Professor of Pharmaceutics at the University of Cincinnati. Mark received his pharmacy degree and PhD in pharmaceutics from the University of Iowa.

The second obstacle feeds off the lack of education. It is the hype or the mainstream narrative that positions AI as a trope of a magic bullet in an almost far-reaching futuristic sense. Lack of understanding leads to misconception, which halts innovative thinking. The overpromise of AI in science leads people to use it or idealise methods of using it that do not complement the technology itself or the industries it could benefit. The weight and importance of tactical and thoughtful implementation that considers science first, allowing AI to act as a collaborator and not a replacement, is immense. There is a fine line between achieving the greatness that AI has in store for us and spoiling it.

Improved education should prevent the hype and change the narrative over time. These two go hand-in-hand. The reality is that new technology will not replace scientific rigor; it will support it. Subsequently, scientific rigor will support and improve the technology.

Another point that has emerged visibly in the last year is how AI-specific companies talk about their capabilities as they relate to drug discovery. Nearly all are trying to differentiate what is possible, positioning proprietary data, software and technology implementations as key aspects of what will lead to new discoveries.

What I have learned is that it is not necessarily what you build or the data you can access but how you approach the problem. This again goes back to a severe need to partner technologists with drug discovery experts.

An example of a good case study for AI usage in the drug discovery process is that today, we can build *in silico* models of many diseases using vast amounts of genomic, phenotypic and chemistry data. All that data can be accessed widely and inexpensively. If we use AI in that process, we can make the data incredibly robust and efficient but only if the scientists inform the data being used. Then, we can use computational methods and algorithms to identify disease features that discovery methods commonly miss due to their dependence on a single predefined hypothesis.

These multiple disease features can be cross-referenced against a library of drug and drug-like molecules and rank those based on success factors defined by the scientists, including predicted efficacy and safety signals. This level of progress would take years using traditional methods but by integrating technology, we can achieve this in a matter of weeks. However, if this process is siloed, where the scientist goes about their usual means and the technologist alone defines the parameters, data will get lost. I have fully seen the benefits of integration in this sense and it is remarkable.

The potential of AI multiplies when paired with better education and integration. We have seen new technology approaches such as AI drive substantial success in finding new treatments that have proven successful in pre-clinical research. I have personally worked on many in the past two years. Today, we stand at a precipice and beyond that is almost certainly a future where the technologists, biologists, pharmacologists, medical experts and others will work in a far more integrated fashion to change drug discovery for the better.

I encourage our industry to look past the hype and instead learn about the actual potential of technology and AI as it specifically relates to drug discovery. I truly believe once those obstacles are overcome, the integration between technologists and scientists will vastly improve. Successful integration means more breakthroughs for patients that need our help.

BIOIVT
ELEVATING SCIENCE®

Millions of Data Points, Endless AI Possibilities

Data and Histology Images from Over 1 Million Biospecimens

- Board-certified confirmed diagnoses, ensuring digital images are representative of clinical disease states
- Aperio full-slide images that integrate into machine-learning–based image analyses
- Over 200 data points, including patient outcomes
- Standardized collection protocols

For more information visit Info.BioIVT.com/AI-Solutions

North America & Asia Pacific
516-483-1196
@customerservice@bioivt.com
PO Box 770, Hicksville NY 11802-0770, U.S.A.

Europe, Middle East & Africa
44 1444 707333
@cseurope@bioivt.com
West Sussex RH15 9TN, U.K.